Solving linear systems: direct methods

Two different approaches

Solve $Ax = b$

Direct methods:

- Deterministic
- Exact up to machine precision
- Expensive (in time and space)

Iterative methods:

- Only approximate
- Cheaper in space and (possibly) time
- Convergence not guaranteed

Really bad example of direct method

Cramer's rule
write $|A|$ for determinant, then

$$x_i = \begin{vmatrix} a_{11} & a_{12} & \dots & a_{1i-1} & b_1 & a_{1i+1} & \dots & a_{1n} \\ a_{21} & & \dots & & b_2 & & \dots & a_{2n} \\ \vdots & & & & \vdots & & & \vdots \\ a_{n1} & & \dots & & b_n & & \dots & a_{nn} \end{vmatrix} / |A|$$

Time complexity $O(n!)$

Gaussian elimination

Example

$$\begin{pmatrix} 6 & -2 & 2 \\ 12 & -8 & 6 \\ 3 & -13 & 3 \end{pmatrix} x = \begin{pmatrix} 16 \\ 26 \\ -19 \end{pmatrix}$$

$$\left[\begin{array}{ccc|c} 6 & -2 & 2 & 16 \\ 12 & -8 & 6 & 26 \\ 3 & -13 & 3 & -19 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} 6 & -2 & 2 & 16 \\ 0 & -4 & 2 & -6 \\ 0 & -12 & 2 & -27 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} 6 & -2 & 2 & 16 \\ 0 & -4 & 2 & -6 \\ 0 & 0 & -4 & -9 \end{array}\right]$$

Solve x_3, then x_2, then x_1

$6, -4, -4$ are the 'pivots'

Pivoting

If a pivot is zero, exchange that row and another.
(there is always a row with a nonzero pivot if the matrix is nonsingular)
best choice is the largest possible pivot
in fact, that's a good choice even if the pivot is not zero

Roundoff control

Consider

$$\begin{pmatrix} \epsilon & 1 \\ 1 & 1 \end{pmatrix} x = \begin{pmatrix} 1+\epsilon \\ 2 \end{pmatrix}$$

with solution $x = (1,1)^t$

Ordinary elimination:

$$\begin{pmatrix} \epsilon & 1 \\ 0 & (1-\frac{1}{\epsilon}) \end{pmatrix} x = \begin{pmatrix} 1 \\ 2-\frac{1}{\epsilon} \end{pmatrix}$$

$$\Rightarrow x_2 = \frac{2-\frac{1}{\epsilon}}{1-\frac{1}{\epsilon}} \Rightarrow x_1 = \frac{1-x_2}{\epsilon}$$

Roundoff 2

If $\epsilon < \epsilon_{\text{mach}}$, then $2 - 1/\epsilon = -1/\epsilon$ and $1 - 1/\epsilon = -1/\epsilon$, so

$$x_2 = \frac{2 - \frac{1}{\epsilon}}{1 - \frac{1}{\epsilon}} = 1, \Rightarrow x_1 = \frac{1 - x_2}{\epsilon} = 0$$

Roundoff 3

Pivot first:

$$\begin{pmatrix} 1 & 1 \\ \epsilon & 1 \end{pmatrix} x = \begin{pmatrix} 2 \\ 1 \end{pmatrix} \Rightarrow \begin{pmatrix} 1 & 1 \\ 0 & 1-\epsilon \end{pmatrix} x = \begin{pmatrix} 2 \\ 1-2\epsilon \end{pmatrix}$$

If ϵ very small:

$$x_1 = \frac{1-2\epsilon}{1-\epsilon} = 1, \qquad x_2 = 2 - x_1 = 1$$

LU factorization

Same example again:

$$A = \begin{pmatrix} 6 & -2 & 2 \\ 12 & -8 & 6 \\ 3 & -13 & 3 \end{pmatrix}$$

2nd row minus $2\times$ first; 3rd row minus $1/2\times$ first; equivalent to

$$L_1 A x = L_1 b, \qquad L_1 = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -1/2 & 0 & 1 \end{pmatrix}$$

LU 2

Next step: $L_2 L_1 A x = L_2 L_1 b$ with

$$L_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -3 & 1 \end{pmatrix}$$

Define $U = L_2 L_1 A$, then $A = L_1^{-1} L_2^{-1} U$
'LU factorization'

LU 3

Observe:

$$L_1 = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -1/2 & 0 & 1 \end{pmatrix} \qquad L_1^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 1/2 & 0 & 1 \end{pmatrix}$$

Likewise

$$L_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -3 & 1 \end{pmatrix} \qquad L_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 3 & 1 \end{pmatrix}$$

Even more remarkable:

$$L_1^{-1} L_2^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 1/2 & 3 & 1 \end{pmatrix}$$

Can be computed in place! (pivoting?)

Solve LU system

$Ax = b \longrightarrow LUx = b$ solve in two steps:
$Ly = b$, and $Ux = y$

Forward sweep:

$$\begin{pmatrix} 1 & & & \emptyset & \\ \ell_{21} & 1 & & & \\ \ell_{31} & \ell_{32} & 1 & & \\ \vdots & & \ddots & & \\ \ell_{n1} & \ell_{n2} & & \cdots & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \\ \vdots \\ b_n \end{pmatrix}$$

$$y_1 = b_1, \quad y_2 = b_2 - \ell_{21} y_1, \ldots$$

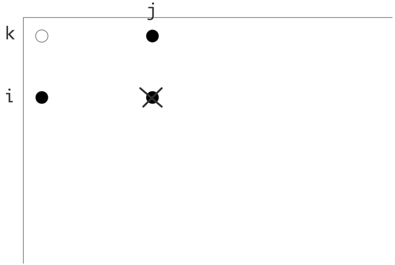
Solve LU 2

Backward sweep:

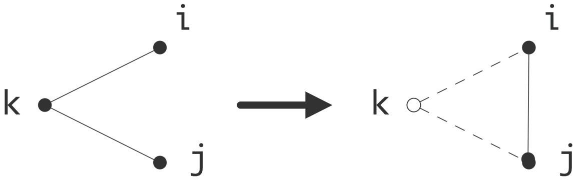
$$\begin{pmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ & u_{22} & \dots & u_{2n} \\ & & \ddots & \vdots \\ \emptyset & & u_{nn} & \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

$$x_n = u_{nn}^{-1} y_n, \quad x_{n-1} = u_{n-1n-1}^{-1}(y_{n-1} - u_{n-1n} x_n), \dots$$

Graph theory of sparse elimination



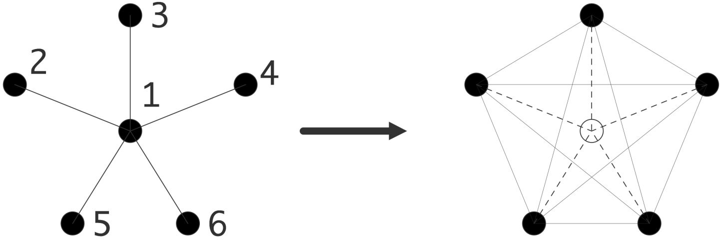
$$a_{ij} \leftarrow a_{ij} - a_{ik} a_{kk}^{-1} a_{kj}$$



Fill-in

Fill-in: index (i, j) where $a_{ij} = 0$ but $\ell_{ij} \neq 0$ or $u_{ij} \neq 0$.

Fill-in is a function of ordering



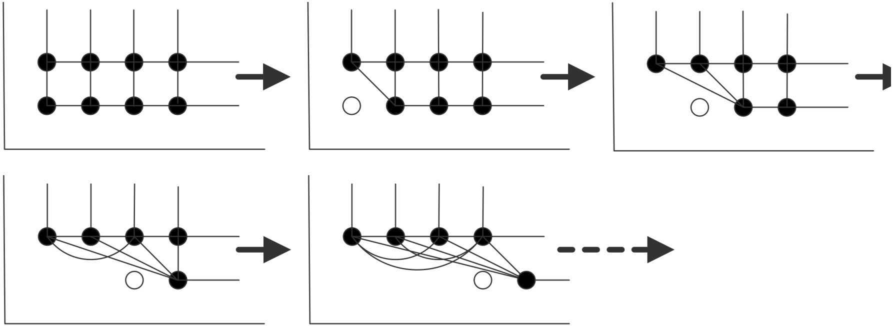
$$\begin{pmatrix} * & * & \cdots & * \\ * & * & & \emptyset \\ \vdots & & \ddots & \\ * & \emptyset & & * \end{pmatrix}$$

After factorization the matrix is dense.
Can this be permuted?

LU of a sparse matrix

$$
\left(\begin{array}{ccccc|ccc}
4 & -1 & 0 & \dots & & -1 & & \\
-1 & 4 & -1 & 0 & \dots & 0 & -1 & \\
 & \ddots & \ddots & \ddots & & & \ddots & \\
\hline
-1 & 0 & \dots & & & 4 & -1 & \\
0 & -1 & 0 & \dots & & -1 & 4 & -1
\end{array}\right)
$$

$$
\Rightarrow \left(\begin{array}{c|cccc|ccc}
4 & -1 & 0 & \dots & & -1 & & \\
\hline
 & 4-\frac{1}{4} & -1 & 0 & \dots & -1/4 & -1 & \\
 & \ddots & \ddots & \ddots & & & \ddots & \\
\hline
 & -1/4 & \dots & & & 4-\frac{1}{4} & -1 & \\
 & -1 & 0 & \dots & & -1 & 4 & -1
\end{array}\right)
$$



Remaining matrix has a dense leading block

Fill-in during LU

2D BVP: Ω is $n \times n$, gives matrix of size $N = n^2$, with bandwidth n.

Matrix storage $O(N)$

LU storage $O(N^{3/2})$

LU factorization work $O(N^2)$